catena-Poly[[diaquacadmium(II)]-μ_2-3-(4-carboxylatophenyl)propionato]

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In the title compound, $[Cd(C_{10}H_8O_4)(H_2O)_2]_n$, the Cd^{II} cation is coordinated in a distorted trigonal–prismatic fashion. 3-(4-Carboxyphenyl)propionate (cpp) ligands connect the Cd^{II} cations into zigzag $[Cd(cpp)(H_2O)_2]_n$ coordination polymer chains, which are oriented parallel to [101]. The chains aggregate into supramolecular layers oriented parallel to $(10\bar{1})$ by means of O—H···O hydrogen bonding between bound water molecules and ligating cpp carboxylate O atoms. The layers stack in an *ABAB* pattern along [100] *via* other O—H···O hydrogen-bonding mechanisms also involving the bound water molecules. The crystal studied was an inversion twin.

3D view	Chemical scheme
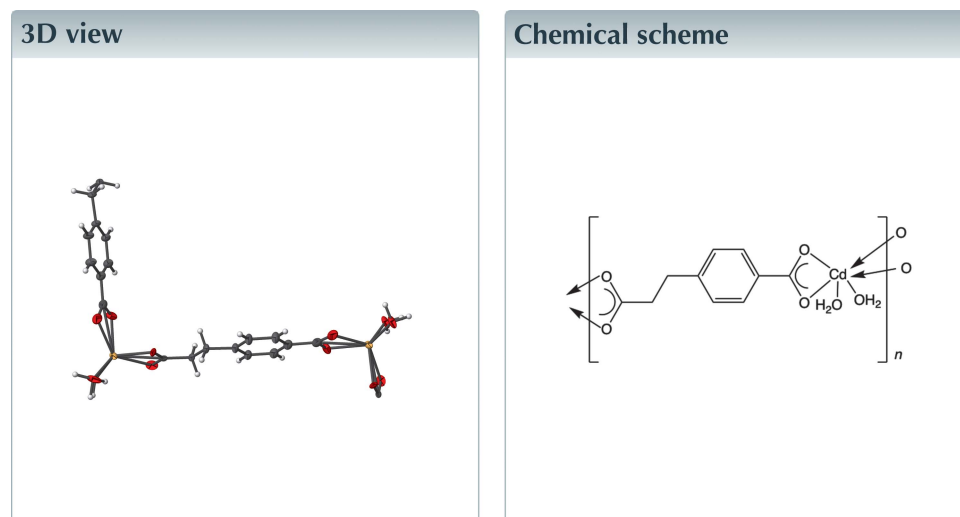
Structure description

The title compound was isolated during an exploratory synthetic effort aiming to produce a cadmium coordination polymer containing both 3-(4-carboxyphenyl)propionate (cpp) and butane-(1,4-diyl)dinicotinamide (bbn) ligands. Cadmium camphorate coordination polymers containing the bbn ligand or other related dipyridylamides have shown intriguing and diverse topologies (Przybyla & LaDuca, 2018).

The asymmetric unit of the title compound contains a Cd^{II} cation, a cpp ligand, and two bound water molecules (O5, O6). The Cd^{II} cation is coordinated in a {CdO₆} trigonal prismatic fashion, with two bound water molecules and chelating carboxylate groups belonging to two different cpp ligands. An ellipsoid plot of the coordination environment and complete ligand set is shown in Fig. 1. The bis(bidentate) cpp ligands form $[Cd(cpp)(H_2O)_2]_n$ zigzag coordination polymer chains oriented parallel [101] (Fig. 2). Within a chain, the Cd···Cd distance through a ligand measures 13.480 (2) Å.

The $[Cd(cpp)(H_2O)_2]_n$ zigzag chains construct supramolecular layers oriented parallel $(10\bar{1})$ by means of O—H···O hydrogen bonding (Table 1) between bound water mol-
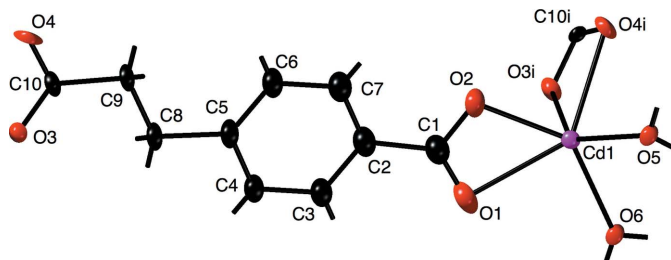
Figure 1
The coordination environment of the Cd^{II} atom, showing trigonal–prismatic coordination. Displacement ellipsoids are drawn at the 50% probability level. H atom positions are shown as sticks. [Symmetry code: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$].

ecules and ligating cpp carboxylate oxygen atoms (Fig. 3) The O···O distance across these hydrogen bonds measure 2.67 (2) and 2.735 (18) Å. The supramolecular layers in turn stack in an *ABAB* pattern along the *a*-axis direction (Fig. 4), mediated by O—H···O hydrogen bonding between bound water molecules and other ligated cpp carboxylate oxygen atoms with a O···O distance of 2.692 (16) Å.

Synthesis and crystallization

Cd(NO$_3$)$_2$·4H$_2$O (114 mg, 0.37 mmol), 3-(4-carboxyphenyl)propionic acid (72 mg, 0.37 mmol), butane-(1,4-diyl)dinicotinamide (110 mg, 0.37 mmol) and 0.75 ml of a 1.0 *M* NaOH solution were placed into 10 ml distilled water in a Teflon-lined acid digestion bomb. The bomb was sealed and heated in an oven at 393 K for 2 d, and then cooled slowly to 273 K. Colourless crystals of the title complex (51 mg, 41%
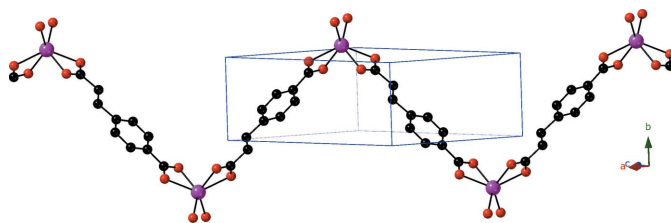

Figure 2
[Cd(cpp)(H$_2$O)$_2$]$_n$ coordination polymer chain in the title compound, oriented parallel [101].
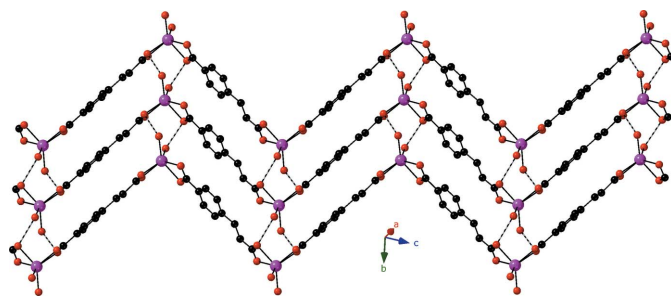

Figure 3
Supramolecular layer in the title compound, oriented parallel ($10\bar{1}$). The O—H···O hydrogen-bonding interactions between adjacent chain submotifs are shown as dashed lines

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6A···O4^i	0.97	2.28	2.653 (15)	102
O6—H6B···O3^{ii}	0.98	1.76	2.735 (18)	176
O5—H5A···O1^{iii}	0.90	1.87	2.692 (16)	151
O5—H5B···O2^{iv}	0.90	2.46	2.67 (2)	94

Symmetry codes: (i) $x, -y + 1, z - \frac{1}{2}$; (ii) $x - \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$; (iii) $x - \frac{1}{2}, y + \frac{1}{2}, z$; (iv) $x, y + 1, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	[Cd(C$_{10}$H$_8$O$_4$)(H$_2$O)$_2$)]
M_r	340.60
Crystal system, space group	Monoclinic, *Cc*
Temperature (K)	173
a, b, c (Å)	11.91424 (16), 5.27697 (7), 18.0006 (3)
β (°)	100.2906 (7)
V (Å^3)	1113.51 (3)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	15.89
Crystal size (mm)	$0.17 \times 0.15 \times 0.04$
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.497, 0.754
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7603, 2127, 2032
R_{int}	0.034
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.065, 1.09
No. of reflections	2127
No. of parameters	139
No. of restraints	63
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.63, −0.49
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.45 (3)

Computer programs: *COSMO* (Bruker, 2009), *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

yield based on Cd) were isolated after washing with distilled water and acetone, and drying in air.
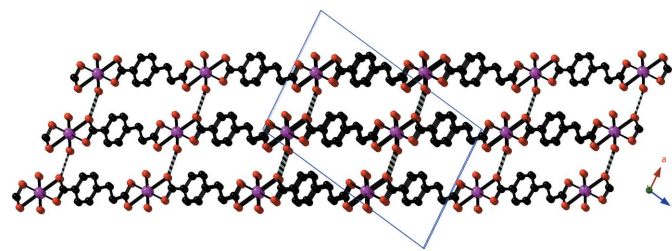

Figure 4
ABA parallel stacking of supramolecular layer motifs in the title compound along [100], mediated by interlayer O—H···O interactions, which are shown as dashed lines.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystal studied was an inversion twin with a refined Flack parameter (Flack, 1983) of 0.45 (3); the structure was best solved and refined in the non-centrosymmetric space group *Cc*. Attempts at refinement of the structure in the centrosymmetric space group *C*2/*c* resulted in disorder and an inability to refine the anisotropic displacement parameters properly.

Acknowledgements

We thank Dr G. Looks for helpful discussion.

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full crystallographic data

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Crystal data

$[Cd(C_{10}H_8O_4)(H_2O)_2]$	$F(000) = 672$
$M_r = 340.60$	$D_x = 2.032$ Mg m^{-3}
Monoclinic, Cc	Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
$a = 11.91424$ (16) Å	Cell parameters from 6487 reflections
$b = 5.27697$ (7) Å	$\theta = 5.0–72.1°$
$c = 18.0006$ (3) Å	$\mu = 15.89$ mm^{-1}
$\beta = 100.2906$ (7)°	$T = 173$ K
$V = 1113.51$ (3) Å^3	Plate, colourless
$Z = 4$	$0.17 \times 0.15 \times 0.04$ mm

Data collection

Bruker APEXII CCD diffractometer	7603 measured reflections
Radiation source: sealed tube	2127 independent reflections
Graphite monochromator	2032 reflections with $I > 2\sigma(I)$
Detector resolution: 8.36 pixels mm^{-1}	$R_{int} = 0.034$
ω and φ scans	$\theta_{max} = 72.2°$, $\theta_{min} = 5.0°$
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)	$h = -14 \rightarrow 14$
	$k = -6 \rightarrow 6$
	$l = -22 \rightarrow 21$
$T_{min} = 0.497$, $T_{max} = 0.754$	

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.025$	$w = 1/[\sigma^2(F_o^2) + (0.0313P)^2 + 4.2565P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.065$	
$S = 1.09$	$(\Delta/\sigma)_{max} < 0.001$
2127 reflections	$\Delta\rho_{max} = 0.63$ e Å^{-3}
139 parameters	$\Delta\rho_{min} = -0.48$ e Å^{-3}
63 restraints	Absolute structure: Refined as an inversion twin
Primary atom site location: dual	Absolute structure parameter: 0.45 (3)

Special details

Experimental. Data was collected using a BRUKER CCD (charge coupled device) based diffractometer equipped with an Oxford low-temperature apparatus operating at 173 K. A suitable crystal was chosen and mounted on a nylon loop using Paratone oil. Data were measured using omega and phi scans of 1.0° per frame for 30 s. The total number of images were based on results from the program COSMO where redundancy was expected to be 4 and completeness to 0.83Å to 100%. Cell parameters were retrieved using APEX II software and refined using SAINT on all observed reflections.Data reduction was performed using the SAINT software which corrects for Lp. Scaling and absorption corrections were applied using SADABS6 multi-scan technique, supplied by George Sheldrick. The structure was solved by the direct method using the SHELXT program and refined by least squares method on F2, SHELXL, incorporated in OLEX2.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The structure was refined by Least Squares using version 2014/6 of XL (Sheldrick, 2008) incorporated in Olex2 (Dolomanov *et al.*, 2009). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cd1	0.5908 (3)	1.12031 (6)	0.6165 (2)	0.01947 (14)
O1	0.7708 (10)	0.943 (3)	0.6755 (7)	0.036 (3)
O2	0.6147 (12)	0.830 (3)	0.7140 (9)	0.029 (3)
O4	0.9084 (8)	−0.445 (3)	1.0590 (7)	0.030 (2)
O6	0.6909 (9)	1.4162 (19)	0.5733 (6)	0.0289 (8)
H6A	0.748862	1.495109	0.610632	0.043*
H6B	0.649566	1.569403	0.554435	0.043*
O3	1.0656 (11)	−0.334 (2)	1.0209 (8)	0.022 (3)
O5	0.4894 (8)	1.433 (2)	0.6558 (6)	0.0289 (8)
H5A	0.416242	1.387459	0.652929	0.043*
H5B	0.484777	1.566549	0.624244	0.043*
C9	0.8830 (8)	−0.1225 (14)	0.9731 (5)	0.0245 (13)
H9A	0.847794	−0.010297	1.006576	0.029*
H9B	0.820939	−0.212517	0.939340	0.029*
C1	0.7208 (13)	0.799 (3)	0.7186 (8)	0.0320 (17)
C2	0.7729 (5)	0.5954 (12)	0.7742 (4)	0.0319 (13)
C7	0.7093 (4)	0.4494 (14)	0.8159 (4)	0.0339 (13)
H7	0.629328	0.475108	0.810536	0.041*
C6	0.7627 (5)	0.2659 (14)	0.8653 (4)	0.0316 (12)
H6	0.719234	0.166173	0.893751	0.038*
C5	0.8797 (5)	0.2284 (12)	0.8731 (4)	0.0285 (11)
C4	0.9433 (4)	0.3743 (10)	0.8314 (4)	0.0290 (11)
H4	1.023238	0.348644	0.836746	0.035*
C3	0.8899 (5)	0.5578 (10)	0.7820 (3)	0.0305 (11)
H3	0.933335	0.657580	0.753531	0.037*
C8	0.9502 (7)	0.0358 (18)	0.9261 (5)	0.0270 (12)
H8A	0.988763	−0.079726	0.895392	0.032*
H8B	1.010205	0.128652	0.960705	0.032*

C10	0.9590 (12)	−0.313 (2)	1.0202 (7)	0.0218 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.01434 (19)	0.01525 (19)	0.0281 (2)	0.0000 (4)	0.00181 (13)	0.0005 (4)
O1	0.026 (5)	0.037 (6)	0.041 (7)	0.013 (6)	−0.008 (4)	−0.010 (7)
O2	0.029 (7)	0.020 (5)	0.038 (7)	0.011 (5)	0.008 (5)	0.002 (6)
O4	0.007 (4)	0.032 (6)	0.052 (7)	−0.007 (5)	0.005 (4)	−0.006 (7)
O6	0.0179 (13)	0.0186 (17)	0.052 (2)	0.003 (3)	0.0123 (13)	0.016 (4)
O3	0.019 (6)	0.021 (5)	0.021 (6)	−0.003 (4)	−0.009 (4)	0.007 (5)
O5	0.0179 (13)	0.0186 (17)	0.052 (2)	0.003 (3)	0.0123 (13)	0.016 (4)
C9	0.025 (3)	0.017 (2)	0.026 (3)	0.009 (2)	−0.010 (2)	−0.002 (2)
C1	0.033 (3)	0.029 (3)	0.030 (3)	0.005 (3)	−0.006 (3)	−0.006 (3)
C2	0.033 (2)	0.029 (2)	0.030 (2)	0.007 (2)	−0.004 (2)	−0.002 (2)
C7	0.036 (3)	0.030 (2)	0.032 (2)	0.005 (2)	−0.005 (2)	0.001 (2)
C6	0.035 (3)	0.026 (2)	0.029 (2)	0.006 (2)	−0.007 (2)	0.0025 (19)
C5	0.032 (2)	0.0232 (19)	0.0263 (19)	0.007 (2)	−0.006 (2)	0.0050 (17)
C4	0.029 (2)	0.028 (2)	0.028 (2)	0.006 (2)	0.000 (2)	0.0090 (19)
C3	0.030 (2)	0.031 (2)	0.029 (2)	0.006 (2)	0.002 (2)	0.008 (2)
C8	0.028 (2)	0.021 (2)	0.027 (2)	0.008 (2)	−0.008 (2)	0.004 (2)
C10	0.021 (3)	0.014 (3)	0.026 (3)	0.008 (3)	−0.010 (3)	−0.009 (3)

Geometric parameters (Å, º)

Cd1—O1	2.405 (13)	C9—C8	1.515 (12)
Cd1—O2	2.309 (16)	C9—C10	1.509 (12)
Cd1—O4[i]	2.418 (12)	C1—C2	1.525 (11)
Cd1—O6	2.190 (11)	C2—C7	1.3900
Cd1—O3[i]	2.269 (13)	C2—C3	1.3900
Cd1—O5	2.235 (12)	C7—H7	0.9500
Cd1—C10[i]	2.670 (11)	C7—C6	1.3900
O1—C1	1.30 (2)	C6—H6	0.9500
O2—C1	1.26 (2)	C6—C5	1.3900
O4—C10	1.22 (2)	C5—C4	1.3900
O6—H6A	0.9673	C5—C8	1.537 (7)
O6—H6B	0.9755	C4—H4	0.9500
O3—C10	1.27 (2)	C4—C3	1.3900
O5—H5A	0.8979	C3—H3	0.9500
O5—H5B	0.8986	C8—H8A	0.9900
C9—H9A	0.9900	C8—H8B	0.9900
C9—H9B	0.9900		
O1—Cd1—O4[i]	134.65 (17)	C10—C9—H9B	109.5
O1—Cd1—C10[i]	115.2 (5)	C10—C9—C8	110.9 (8)
O2—Cd1—O1	55.1 (6)	O1—C1—C2	128.8 (13)
O2—Cd1—O4[i]	92.9 (5)	O2—C1—O1	116.4 (13)
O2—Cd1—C10[i]	94.0 (5)	O2—C1—C2	114.8 (14)

O4ⁱ—Cd1—C10ⁱ	27.2 (5)	C7—C2—C1	123.2 (8)
O6—Cd1—O1	86.2 (5)	C7—C2—C3	120.0
O6—Cd1—O2	137.9 (5)	C3—C2—C1	116.8 (8)
O6—Cd1—O4ⁱ	128.7 (5)	C2—C7—H7	120.0
O6—Cd1—O3ⁱ	102.2 (5)	C6—C7—C2	120.0
O6—Cd1—O5	86.83 (15)	C6—C7—H7	120.0
O6—Cd1—C10ⁱ	119.8 (4)	C7—C6—H6	120.0
O3ⁱ—Cd1—O1	93.6 (5)	C7—C6—C5	120.0
O3ⁱ—Cd1—O2	96.73 (15)	C5—C6—H6	120.0
O3ⁱ—Cd1—O4ⁱ	55.5 (5)	C6—C5—C8	125.7 (4)
O3ⁱ—Cd1—C10ⁱ	28.4 (5)	C4—C5—C6	120.0
O5—Cd1—O1	129.6 (5)	C4—C5—C8	114.3 (4)
O5—Cd1—O2	104.5 (4)	C5—C4—H4	120.0
O5—Cd1—O4ⁱ	85.6 (4)	C5—C4—C3	120.0
O5—Cd1—O3ⁱ	136.6 (4)	C3—C4—H4	120.0
O5—Cd1—C10ⁱ	111.5 (5)	C2—C3—H3	120.0
C1—O1—Cd1	91.3 (9)	C4—C3—C2	120.0
C1—O2—Cd1	96.9 (11)	C4—C3—H3	120.0
C10—O4—Cd1ⁱⁱ	88.0 (7)	C9—C8—C5	115.3 (6)
Cd1—O6—H6A	115.2	C9—C8—H8A	108.5
Cd1—O6—H6B	116.2	C9—C8—H8B	108.5
H6A—O6—H6B	98.0	C5—C8—H8A	108.5
C10—O3—Cd1ⁱⁱ	93.6 (10)	C5—C8—H8B	108.5
Cd1—O5—H5A	110.9	H8A—C8—H8B	107.5
Cd1—O5—H5B	110.7	O4—C10—Cd1ⁱⁱ	64.8 (7)
H5A—O5—H5B	103.0	O4—C10—O3	122.6 (12)
H9A—C9—H9B	108.0	O4—C10—C9	113.2 (12)
C8—C9—H9A	109.5	O3—C10—Cd1ⁱⁱ	58.0 (8)
C8—C9—H9B	109.5	O3—C10—C9	124.2 (13)
C10—C9—H9A	109.5	C9—C10—Cd1ⁱⁱ	173.8 (9)
Cd1—O1—C1—O2	−4.7 (16)	C2—C7—C6—C5	0.0
Cd1—O1—C1—C2	174.9 (14)	C7—C2—C3—C4	0.0
Cd1—O2—C1—O1	4.9 (17)	C7—C6—C5—C4	0.0
Cd1—O2—C1—C2	−174.7 (10)	C7—C6—C5—C8	179.1 (7)
Cd1ⁱⁱ—O4—C10—O3	5.6 (15)	C6—C5—C4—C3	0.0
Cd1ⁱⁱ—O4—C10—C9	−173.6 (9)	C6—C5—C8—C9	−0.1 (10)
Cd1ⁱⁱ—O3—C10—O4	−5.9 (16)	C5—C4—C3—C2	0.0
Cd1ⁱⁱ—O3—C10—C9	173.1 (11)	C4—C5—C8—C9	179.0 (6)
O1—C1—C2—C7	−178.3 (13)	C3—C2—C7—C6	0.0
O1—C1—C2—C3	1 (2)	C8—C9—C10—O4	−180.0 (11)
O2—C1—C2—C7	1.3 (18)	C8—C9—C10—O3	0.9 (17)
O2—C1—C2—C3	−179.0 (12)	C8—C5—C4—C3	−179.2 (7)
C1—C2—C7—C6	179.7 (9)	C10—C9—C8—C5	177.3 (8)
C1—C2—C3—C4	−179.7 (9)		

Symmetry codes: (i) $x-1/2$, $-y+1/2$, $z-1/2$; (ii) $x+1/2$, $-y+1/2$, $z+1/2$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6*A*···O4[iii]	0.97	2.28	2.653 (15)	102
O6—H6*B*···O3[iv]	0.98	1.76	2.735 (18)	176
O5—H5*A*···O1[v]	0.90	1.87	2.692 (16)	151
O5—H5*B*···O2[vi]	0.90	2.46	2.67 (2)	94
C3—H3···O1				

Symmetry codes: (iii) *x*, −*y*+1, *z*−1/2; (iv) *x*−1/2, −*y*+3/2, *z*−1/2; (v) *x*−1/2, *y*+1/2, *z*; (vi) *x*, *y*+1, *z*.